Applied Magnetic Resonance 2002 vol.23 N1, pages 97-104

Low-lying states of trinuclear mixed-valence cluster: [Fe3S4]0

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Abstract

Low-lying energy states of the [Fe3S4]0 cluster have been calculated by taking into account the double exchange, superexchange and vibronic interaction. It was found that the adiabatic potential of the excited state with S = 0 corresponds to the full delocalization of the "excess" charge. From the analysis of experimental data of Mössbauer spectroscopy and the temperature dependence of the magnetic susceptibility the double exchange parameter t ≥ 4000 cm-1 and the vibronic interaction parameter λ2/2k ≥ 2800 cm-1 have been estimated.